PHY 712 Electrodynamics
10-10:50 AM MWF Olin 103

Class notes for Lecture 2:

Reading: Chapter 1 (especially 1.11) in JDJ;

1. Calculation of the electrostatic energy for a finite system
2. Electrostatic energy in terms of electrostatic fields
3. Electrostatic energy of extended systems -- introduction to Ewald summation methods

Physics Colloquium
Thursday, January 12, 2023
4 PM in Olin 101

Professor John Weisel,
U. Pennsylvania,
Perelman School of Medicine

"Blood clot contraction: Mechanisms, pathophysiology, and disease"

(hosts: M. Guthold and S. Baker)

https://physics.wfu.edu/wfu-phy-news/colloquium/seminar-2023-spring/

PHY 712 Electrodynamics

MWF 11-11:50 AM	**Olin 103**	Webpage: **http://www.wfu.edu/~natalie/s22phy712/**

Instructor: Natalie Holzwarth	**Office:**300 OPL	**e-mail:**natalie@wfu.edu

---

Course schedule for Spring 2022

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	JDJ Reading	Topic	HW	Due date
1	Mon: 01/10/2022	Chap. 1 & Appen.	Introduction, units and Poisson equation	#1	01/14/2022
2	Wed: 01/12/2022	Chap. 1	Electrostatic energy calculations	#2	01/19/2022
3	Fri: 01/14/2022	Chap. 1	Electrostatic energy calculations	#3	01/21/2022
	Mon: 01/17/2022		MLK Holiday -- no class		

PHY 712 -- Assignment #2

January 11, 2023

Continue reading Chap. 1 in **Jackson**.

1. Calculate and numerically evaluate the electrostatic energy of the following 5 ion molecule scaled by the factor $(1/(4\pi\varepsilon_0))\ (q^2 / a)$. Comment on the significance of the sign of your result. Note that **x**, **y**, and **z** denote unit vectors in the three Cartesian directions.

   - Charge = -4q   Position = 0
   - Charge = q   Position = (a/2)(**x**+**y**+ **z**)
   - Charge = q   Position = (a/2)(-**x**-**y**+ **z**)
   - Charge = q   Position = (a/2)(**x**-**y**+ **z**)
   - Charge = q   Position = (a/2)(-**x**+**y**+ **z**)

Calculation of the electrostatic energy of a system of charges --

Consider a collection of point charges $\{q_i\}$ located at points $\{\mathbf{r}_i\}$.

The energy to separate these charges to infinity$(\mathbf{r}_i \to \infty\}$ is

$$W = \frac{1}{4\pi\epsilon_0} \sum_{(i,j;i>j)} \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j|}.$$

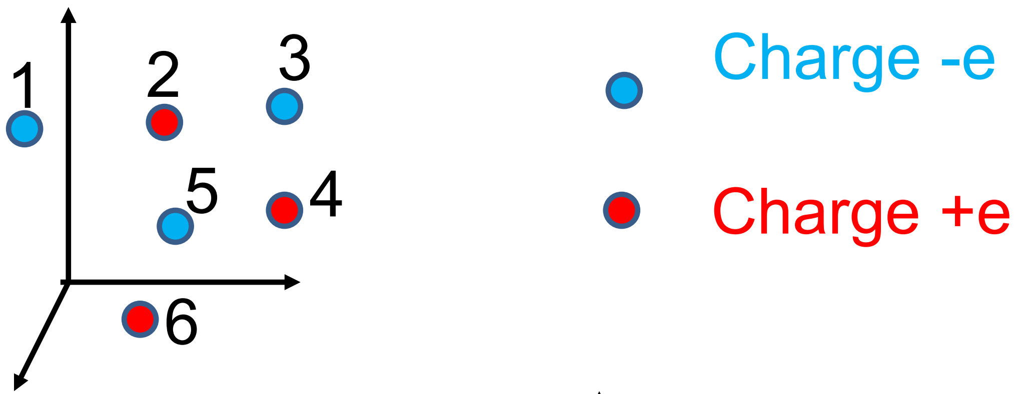
Here the summation is over all pairs of (i, j), excluding $i = j$.

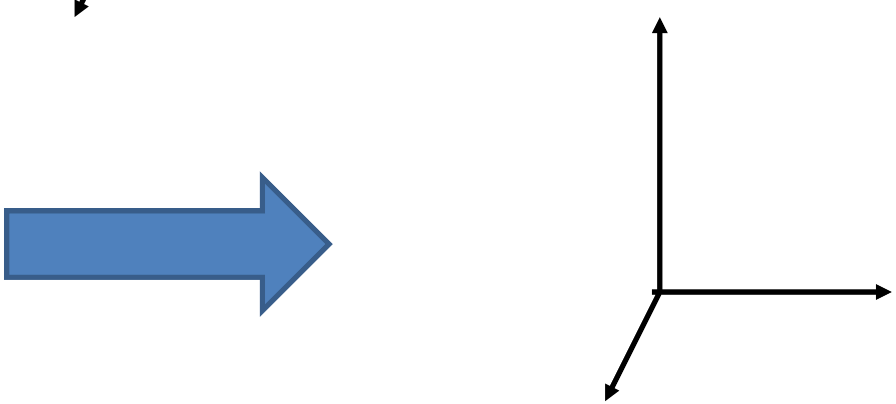
Define $$W_{ij} \equiv \frac{q_i q_j}{4\pi\epsilon_0} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} .$$

$$W = \sum_{(i,j;i>j)} W_{ij}$$

Note that this result is likely to grow in magnitude with increasing numbers of charged particles.

Example finite charge system for which electrostatic energy W can be calculated in a straightforward way





(particles moves off to infinity)

$$W = W_{12} + W_{13} + W_{14} + W_{15} + W_{16} + W_{23} + W_{24} + W_{25} + W_{26}$$
$$+ W_{34} + W_{35} + W_{36} + W_{45} + W_{46} + W_{56}$$

Summary --

Consider a collection of point charges $\{q_i\}$ located at points $\{\mathbf{r}_i\}$.

The energy to separate these charges to infinity$(\mathbf{r}_i \rightarrow \infty\}$ is

$$W = \frac{1}{4\pi\epsilon_0} \sum_{(i,j;i>j)} \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j|}.$$

Here the summation is over all pairs of (i, j), excluding $i = j$.

It is sometimes convenient to sum over all particles and divide by 2 in order to compensate for the double counting:

$$W = \frac{1}{8\pi\epsilon_0} \sum_{i,j;i\neq j} \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j|}.$$

Now the summation is over all i and j, excluding $i = j$.

The energy W scales as the number of particles N. As N $\rightarrow \infty$, the ratio W / N remains well-defined in principle, but difficult to calculate in practice.

Slight digression:

Comment on electrostatic energy evaluation --

When the discrete charge distribution becomes a continuous charge density: $q_i \rightarrow \rho(\mathbf{r})$, the electrostatic energy becomes

$$W = \frac{1}{8\pi\epsilon_0}\int d^3r\, d^3r' \,\frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}.$$

Notice, in this case, it is not possible to exclude the ``self-interaction''.

Electrostatic energy in terms of $\Phi(\mathbf{r})$ and field $\mathbf{E}(\mathbf{r})$:

Previous expression can be rewritten in terms of the electrostatic potential or field:

$$W = \frac{1}{2}\int d^3r\, \rho(\mathbf{r})\Phi(\mathbf{r}) = -\frac{\epsilon_0}{2}\int d^3r \left(\nabla^2\Phi(\mathbf{r})\right)\Phi(\mathbf{r}).$$

$$W = \frac{\epsilon_0}{2}\int d^3r \left|\nabla\Phi(\mathbf{r})\right|^2 = \frac{\epsilon_0}{2}\int d^3r \left|\mathbf{E}(\mathbf{r})\right|^2.$$

Some details --

Electrostatic potential

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0}\int d^3r' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

Electrostatic field

$$\mathbf{E}(\mathbf{r}) = -\nabla\Phi(\mathbf{r})$$

Poisson equation

$$\nabla^2\Phi(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\varepsilon_0}$$

Summary for continuum --
Electrostatic energy

$$W = \frac{1}{8\pi\epsilon_0}\int d^3r\, d^3r' \,\frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}.$$

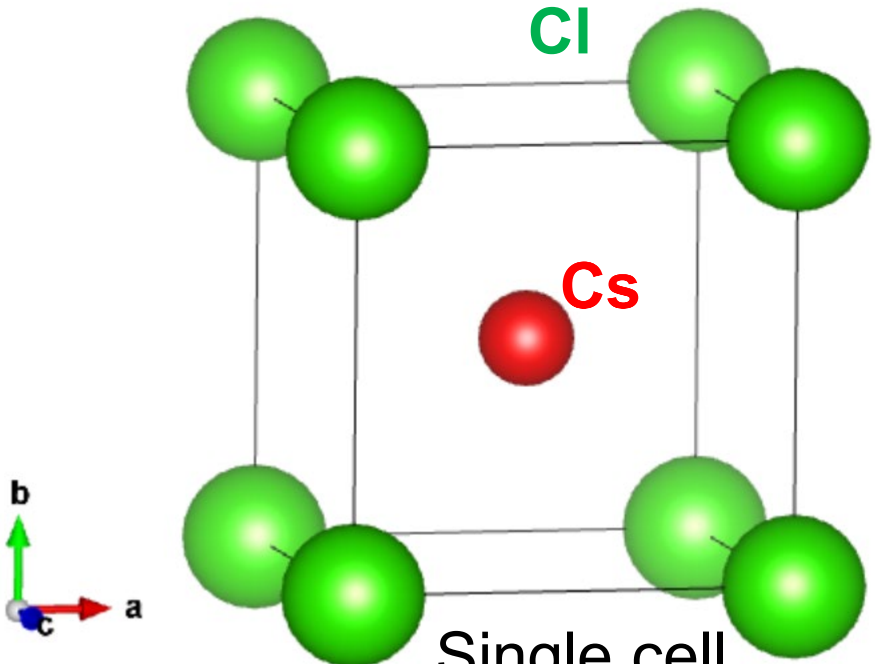
Evaluation of electrostatic energy in terms of potential $\Phi(\mathbf{r})$ and field $\mathbf{E}(\mathbf{r})$:

$$W = \frac{1}{2}\int d^3r\; \rho(\mathbf{r})\Phi(\mathbf{r}) = -\frac{\epsilon_0}{2}\int d^3r\left(\nabla^2\Phi(\mathbf{r})\right)\Phi(\mathbf{r}).$$

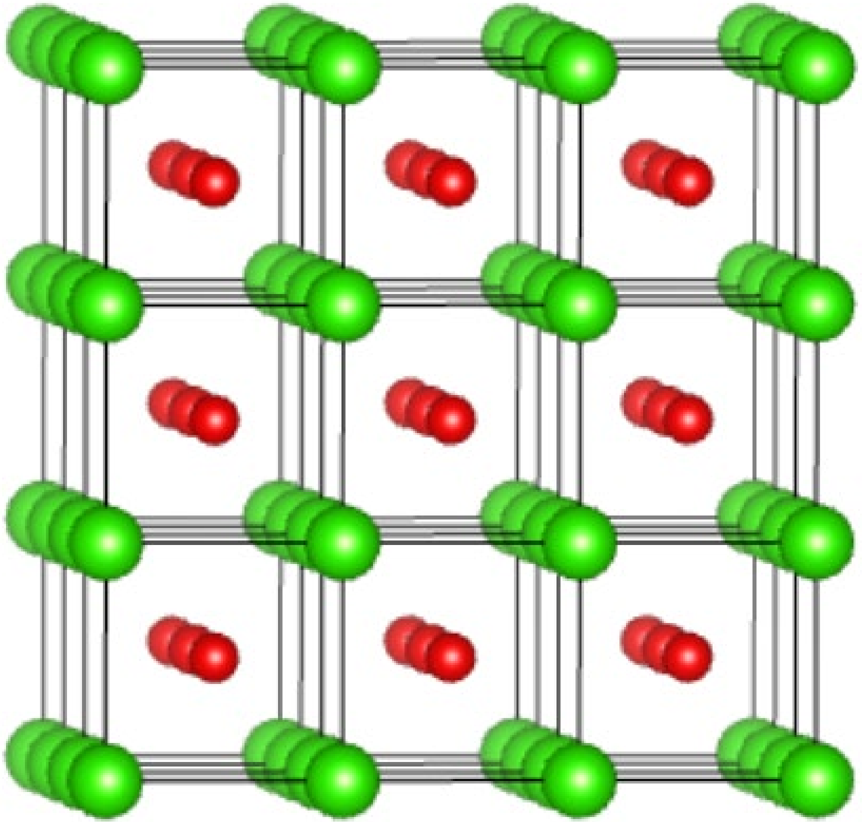
$$W = \frac{\epsilon_0}{2}\int d^3r\left|\nabla\Phi(\mathbf{r})\right|^2 = \frac{\epsilon_0}{2}\int d^3r\left|\mathbf{E}(\mathbf{r})\right|^2.$$

In general, the evaluation of the electrostatic energy of an extended system can be numerically tricky because of the long range nature of the Coulombic forces.

Now consider the electrostatic energy of a periodic crystal of CsCl



Single cell



Multiple cells

In general, the evaluation of the electrostatic energy of an extended system can be numerically tricky because of the long range nature of the Coulombic forces.

However, thanks to very clever mathematicians, it is possible to perform this sort of calculation for periodic systems.

[Ewald, Paul Peter, 1888-1985]

American crystallographer, emigrated from Germany

The direct summation of the electrostatic terms of an infinite ionic system diverges, however using Ewald's ideas the single divergent summation can be represented by two converging summations (plus a few corrections).

The formula that we will derive and use for a lattice with periodic real space translations T and reciprocal space translations G is:

$$\frac{W}{N} = \sum_{\alpha\beta} \frac{q_\alpha q_\beta}{8\pi\varepsilon_0} \left(\frac{4\pi}{\Omega} \sum_{\mathbf{G}\neq\mathbf{0}} \frac{e^{-i\mathbf{G}\cdot\tau_{\alpha\beta}}\ e^{-G^2/\eta}}{G^2} - \sqrt{\frac{\eta}{\pi}}\delta_{\alpha\beta} + {\sum_{\mathbf{T}}}' \frac{\operatorname{erfc}(\frac{1}{2}\sqrt{\eta}|\tau_{\alpha\beta}+\mathbf{T}|)}{|\tau_{\alpha\beta}+\mathbf{T}|} \right) - \frac{4\pi Q^2}{8\pi\varepsilon_0\Omega\eta}$$